Exploiting Non-Native Molecular Arrangements in Binary Ionic Liquids to Enhance Gas Solubility

Utkarsh Kapoor and Jindal Shah [C, S]
School of Chemical Engineering, Oklahoma State University, Stillwater, OK, U.S.A.
jindal.shah@okstate.edu

Ionic liquids are substances that are composed entirely of ions. Negligible vapor pressures and the availability of a large number of cations and anions to tune physicochemical and biological properties for a given chemical process have been the primary drivers for research in this field over the last two decades. A majority of these investigations have focused primarily on elucidating changes in the properties of pure ionic liquids by altering the cation, anion, or substituents on the ions. Another approach to expand the range of available ionic liquids is to form ionic liquid-ionic liquid mixtures. From a thermodynamic point of view, knowledge of the extent of non-ideality for these binary ionic liquid mixtures and the molecular level details enable *a priori* prediction of thermophysical properties of ionic liquid properties. In this presentation, we will show, with the aid of molecular simulations, that the difference in the hydrogen bonding ability of the anions can serve as a metric for the prediction of non-ideality in the binary ionic liquid systems. Such non-idealities are quantified in terms of the local structural organization of anions around the cation. We will further demonstrate that the presence of non-idealities in the local structural organization can be leveraged to obtain CO_2 solubilities higher than those predicted by the ideal behavior.